TITLE:	Development of Superior Sorbents for Separation of CO_2 from Flue Gas at a Wide Temperature Range during Coal Combustion: IC Phase II

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1. ABSTRACT

Program Introduction: Rationale and Objectives

CO_2 is considered as the major greenhouse gas contributing to global warming. The use of metal exchanged low silicon (LSX) faujasites is widely accepted in industry but it is limited by the fact that it can be used for mixtures containing only low concentrations of CO_2. Unfortunately, those sorbents are effective to remove CO_2 from gas mixtures which only contain gases that are less polar than carbon dioxide. Existing sorbents cannot operate at elevated temperatures due to rapid loss of structural stability and regenerability. Moreover, the existing systems are not versatile to be utilized for other processes (i.e. fuel cell applications, purification of H_2 from WGS, membranes, etc.) and they are also very sensitive to poisons and impurities.

Hence, a new generation of sorbents for removal of CO_2 at a wide range of temperatures (30 to 650 ^oC) is needed. The high temperature can be utilized for the CO_2 removal from hot gas streams (flue gas, gas generated from coal gasification, fuel cell applications, etc.). Equally important requirements are the high temperature stability of the sorbents as well as their ability to be regenerated reversibly and restore their performance to the initial levels. Sorbents with high selectivity for CO_2 with respect to other gases of multicomponent mixtures (including gases which are more polar that CO_2) is *a must for* an effective separation. Successful sorbents should have low affinity for water, O_2, N_2, water and they should be tolerant to poisons and should demonstrate ease for adaptability into existing units.

The objectives of this project are:

1) Integrate the synthesis efforts aiming at developing basic and superbasic supports and sorbents. Enhance the knowledge of functionalizing the surface for obtaining the desirable performance.

2) Characterize the synthesized sorbents with numerous state-of-the-art characterization techniques to understand their surface properties and functionality.
3) Direct the synthesis and characterizations toward highly durable systems that will ensure stability for regeneration over many hundred cycles at elevated temperatures and severe operating environments.
4) Use the obtained information as feed-back to design the most effective sorbents. Test these sorbents with gas mixtures containing CO_2, H_2O, air, SO_2, SO_3, H_2, and CO at selected compositions simulating industrial operation.

Accomplishments Achieved during the Current Period of Performance

We have developed high temperature Cs/CaO sorbents **for CO_2 separation with zero affinity for N_2, O_2 and NO**. This is a remarkable property since nitrogen and oxygen consist of more that 80% of the volume of gases leaving a typical coal boiler. Moreover, NO does not interact with our sorbents at high temperatures which is a great advantage.

Moreover, we found that our sorbents have zero or minimal affinity for water depending on the operational conditions. This is another important advantage since water corresponds to more than 10% of the volume of gases leaving the boiler. Experiments with SO_2 showed a permanent attachment of sulfur species on the surface of the sorbent.

We have initiated the synthesis of aerosol made sorbents based on alkali metal/CaO as potential sorbents with superior mechanical properties and stability for operation in cyclic processes.

Plans for the coming year

- Correlate sorption performance with surface characteristics for obtaining a better fundamental understanding.
- Synthesize aerosol CaO-based sorbents. Use Si as dopant to reinforce their structure.
- Continue characterization of the sorbents with modern analytical techniques.
- Continue sorption experiments with the new family of sorbents. Use realistic gas mixtures simulating flue gas composition.

2. LIST OF PUBLISHED JOURNAL ARTICLES, COMPLETED PRESENTATIONS, AND STUDENTS RECEIVING SUPPORT FROM THE GRANT

Journal Articles (peer reviewed)

1) A. Roesch, E.P. Reddy, and P.G. Smirniotis, P. G. "Parametric Study of Cs/CaO sorbents for removal of CO_2 with respect to simulated flue gases at high temperatures", *Gas Separations and Purifications*, in preparation for submission, (2004)

Conference Presentations

1) A. Roesch, E.P. Reddy, and P.G. Smirniotis, P. G. "CO_2 sorbents based on Cs/CaO at high temperatures", *Gas Separations and Purifications*, in preparation for submission, (2004).

Students Receiving Support from the Grant.

Graduate Students:

1) Mr. Bo Sun, graduate student (Ph.D.) in Chemical Engineering
2) Mr. Hong Lu, graduate student (Ph.D.) in Chemical Engineering